

Multi-fluid Model of Exothermic Fields in Explosions

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Multi-fluid Model of Exothermic Fields in Explosions

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1. Formulation

Proposed here is a multi-fluid extension of our multi-component model [1] of unmixed combustion in explosions. We recognize three fluids: *Fuel-F* and *Air-A* forming combustion *Products-P* at thermodynamic equilibrium. We consider the inviscid exothermic-flow limit [2]—where all molecular transport phenomena can be disregarded; thus, the Reynolds number $Re \rightarrow \infty$; the Peclet number for both heat and mass diffusion $Pe \rightarrow \infty$; the Damköhler number $Da \rightarrow \infty$, and the Mach number $Ma > 0$. As is typical of combustion in unmixed systems [3], fuel and air react in stoichiometric proportions σ called *Reactants-R*.

2. Conservation Equations

In the limit of $Re \rightarrow \infty$, the *mixture*— m is governed by the *Gasdynamic Conservation Laws*:

$$\text{Mass:} \quad \partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}) = 0 \quad (1)$$

$$\text{Momentum:} \quad \partial_t \rho_m \mathbf{u} + \nabla \cdot (\rho_m \mathbf{u} \mathbf{u}) = -\nabla p_m \quad (2)$$

$$\text{Energy:} \quad \partial_t \rho_m E_m + \nabla \cdot (\rho_m E_m \mathbf{u}) = [u_p - u_R](1 + \sigma) \dot{\rho}_e \quad (3)$$

where ρ, u, p and \mathbf{u} denote density, internal energy, pressure and velocity vector, respectively, while $E_m \equiv u_m + \mathbf{u} \cdot \mathbf{u} / 2$ and $[u_p - u_R]$ represents the energy transformation from R to P . To evaluate the pressure in fluid K , one needs to know its density and energy (i.e., $p_K = p_K(\rho_K, u_K)$ where $K=F, A, P$); these are obtained from *Mass-Energy Conservation Laws* for each fluid; at $Pe \rightarrow \infty$ they acquire the form

$$F: \quad \partial_t \rho_F + \nabla \cdot (\rho_F \mathbf{u}) = -\dot{\rho}_e \quad \& \quad \partial_t \rho_F u_F + \nabla \cdot (\rho_F u_F \mathbf{u}) = -p_F \nabla \cdot \mathbf{u} - u_F \dot{\rho}_e \quad (4a,b)$$

$$A: \quad \partial_t \rho_A + \nabla \cdot (\rho_A \mathbf{u}) = -\sigma \dot{\rho}_e \quad \& \quad \partial_t \rho_A u_A + \nabla \cdot (\rho_A u_A \mathbf{u}) = -p_A \nabla \cdot \mathbf{u} - u_A \sigma \dot{\rho}_e \quad (5a,b)$$

$$P: \quad \partial_t \rho_P + \nabla \cdot (\rho_P \mathbf{u}) = (1 + \sigma) \dot{\rho}_e \quad \& \quad \partial_t \rho_P u_P + \nabla \cdot (\rho_P u_P \mathbf{u}) = -p_P \nabla \cdot \mathbf{u} + u_P (1 + \sigma) \dot{\rho}_e \quad (6a,b)$$

$$m: \quad \rho_m \equiv \rho_F + \rho_A + \rho_P \quad \& \quad u_m \equiv (\rho_F u_F + \rho_A u_A + \rho_P u_P) / \rho_m \quad (7)$$

Combustion influences these fields only at the *exothermic front-e*, which is a sink ($\dot{\rho}_e$) for F & A and a source for P . The equations are integrated by a higher order Godunov method.

Adaptive Mesh Refinement provides enough mesh resolution to capture the mixing structures on the grid—so no turbulence model is needed [1].

3. Exothermic Front

According to the approximation $Da \rightarrow \infty$, the front [1] is represented as a Dirac delta function, δ , located at the stoichiometric contour, $\mathbf{x}_e(t_e)$:

$$\dot{\rho}_e \equiv \begin{cases} \rho_F \delta(\mathbf{x} - \mathbf{x}_e, t - t_e) & (1 \leq \lambda_e < \infty) \\ 0 & (\lambda = 0, \infty) \\ \rho_A \delta(\mathbf{x} - \mathbf{x}_e, t - t_e) / \sigma & (0 < \lambda_e < 1) \end{cases} \quad (8)$$

where $\lambda(\mathbf{x}, t) \equiv (A - F \text{ ratio}) / \sigma$, which varies throughout the flow field due to mixing.

4. Thermodynamics

Thermodynamic properties of the fluids are displayed in the Le Chatelier diagram (Fig. 1) of

$$W_K \equiv (p\nu)_K / w_{Ai} \quad \& \quad U_K \equiv (u_K - u_{0K}) / C_A w_{Ai} = Q_K + k_K W_K \quad (9)$$

In an exothermic cell, F and A combine in stoichiometric proportions forming a point on *curve-R*; combustion transforms that point to one on *curve-P*. If the system is adiabatic, this transformation occurs initially at constant pressure and enthalpy (point hp), and at the final stage of combustion it occurs at constant energy and volume (point uv).

5. Illustration

This *Model* was used to simulate the combustion of the expanded detonation products from a 1-kg charge of TNT with air in a $V = 16.6\text{-m}^3$ chamber. Figure 2 shows the measured enhancement of pressure due to combustion [4]. The mean (volume-averaged) fluid densities and energies from the simulation are presented in Figs. 3 and 4. The mass fraction of fuel consumed is shown in Fig. 5. The calculated pressure history agrees with data (Fig. 6).

6. Conclusion

Combustion in the *Multi-Fluid Model* is treated material transformations in the Le Chatelier plane (rather than “heat release” found in traditional models). This is the only way to construct a thermodynamically-consistent representation of the fluids. The *exothermic front* provides an extraordinarily sharp representation of turbulent combustion fields—which are normally clouded by a myriad of diffusional effects.

References

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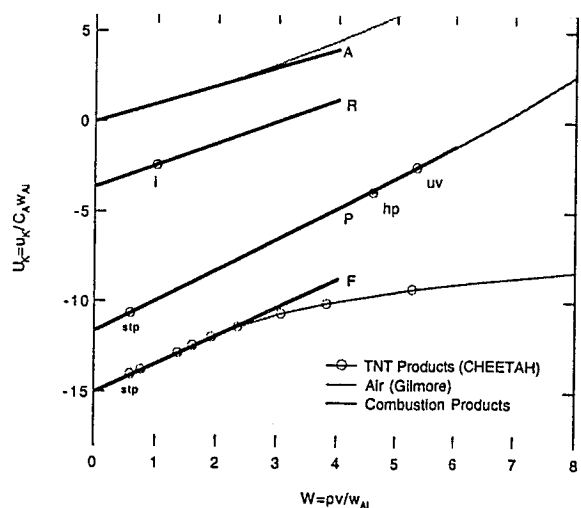


Fig. 1. Le Chatelier diagram for combustion of TNT detonation products in air.

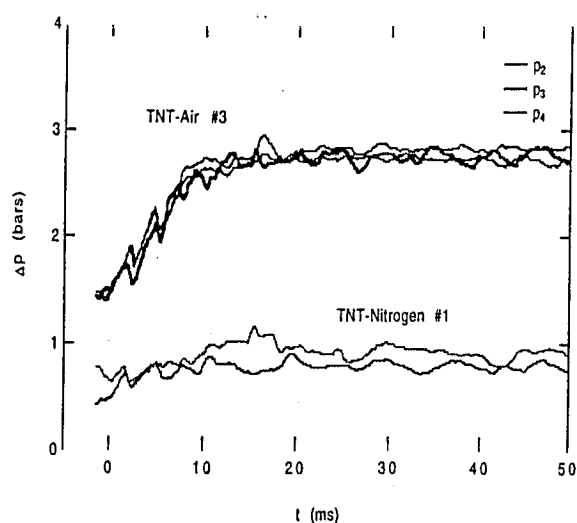


Fig. 2. Mean pressure histories for a 1-kg TNT explosion in air and N_2 ($V=17m^3$).

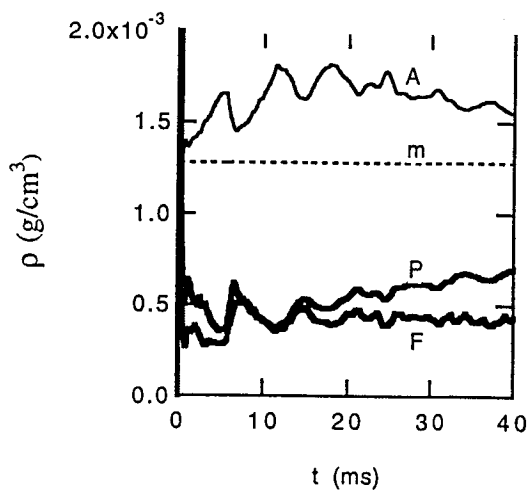


Fig. 3. Mean density histories of the fluids.

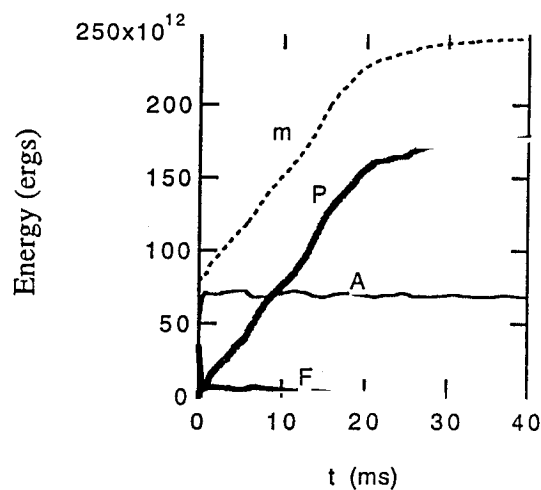


Fig. 4. Mean energy histories of the fluids.

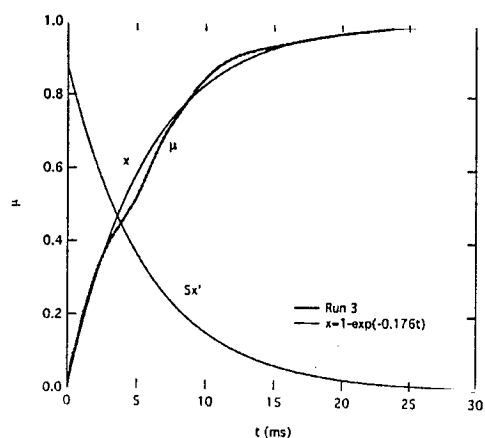


Fig. 5. Mass-fraction of fuel consumed.

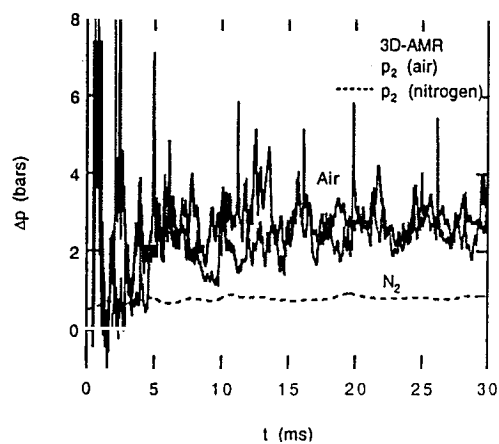


Fig. 6. Pressure history comparison.

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ABSTRACT

A *Multi-fluid Model* is proposed for turbulent combustion in explosions at infinitely-large Reynolds, Peclet & Damköhler numbers. It is based on the *gasdynamic conservation laws* for the mixture, augmented *mass-energy conservation laws* for each fluid (fuel- F , oxidizer- A and products- P). Combustion is treated as material transformations in the Le Chatelier plane—rather than “heat release” found in traditional models. This allows one to construct thermodynamically-consistent representations of the fluids. Such transformations occur at an *exothermic front*—which represents, simultaneously, a *sink* for F & A and *source* of P . The front is represented by a Dirac delta function at the stoichiometric contour in the turbulent field. This *Model* then provides an extraordinarily clear picture of turbulent combustion fields, which are normally clouded by a myriad of diffusional effects.

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